Moving towards supporting real time analysis and manipulation on a molecular level

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Shoaib Sufi, Glen Drinkwater, Louisa Casely-Hayford, Brian Matthews - STFC

October 2010

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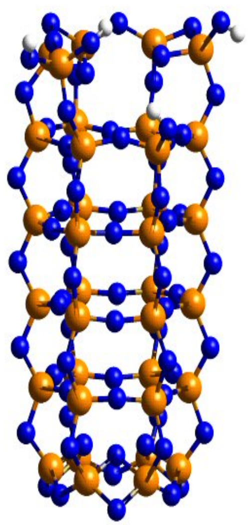
Motivation

- Enabling improved analysis through more complete information, facilitated by allowing users to get rapid access to current and past data, related projects, publications etc.

- Enabling rational design and synthesis of new chemical, biological, and materials systems through integrated molecular scale imaging technologies, real time analysis and manipulation.



Capturing Data and Making it Accessible – STFC 2002-2008

Science & Technology Facilities Council

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UK Science and Technology Facilities Council (STFC)

STFC (formerly CCLRC) facilitates the access to large scale experimental and computational facilities for the UK research community, both through subscriptions to international institutions and by operating a range of world class facilities e.g.:

- **ISIS Neutron and Muon Facility**
- **Daresbury Laboratory Synchrotron**
- **DIAMOND Light Source**
- **Central Laser Facilities**

Science & Technology
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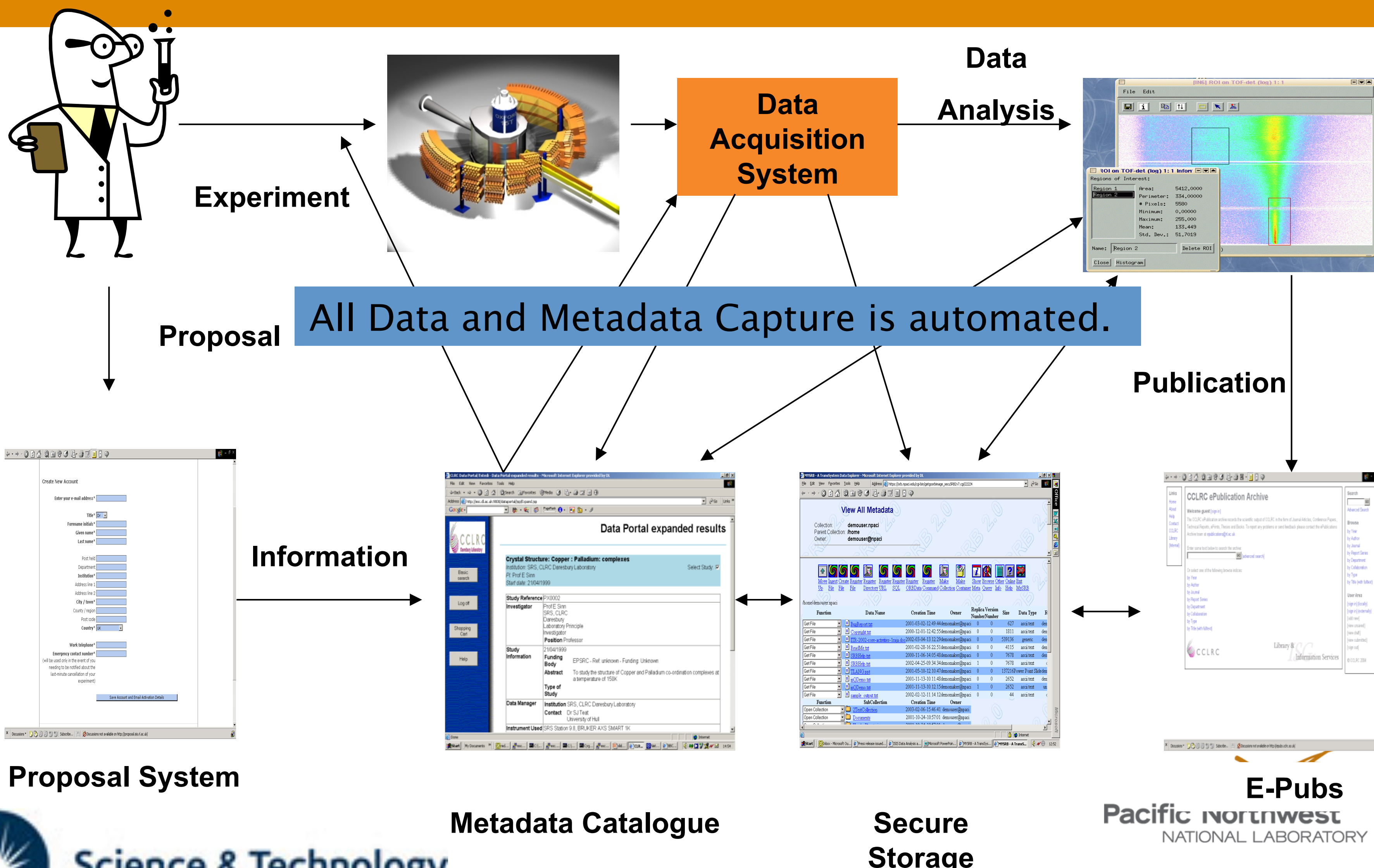
Integrated e-Infrastructure Vision



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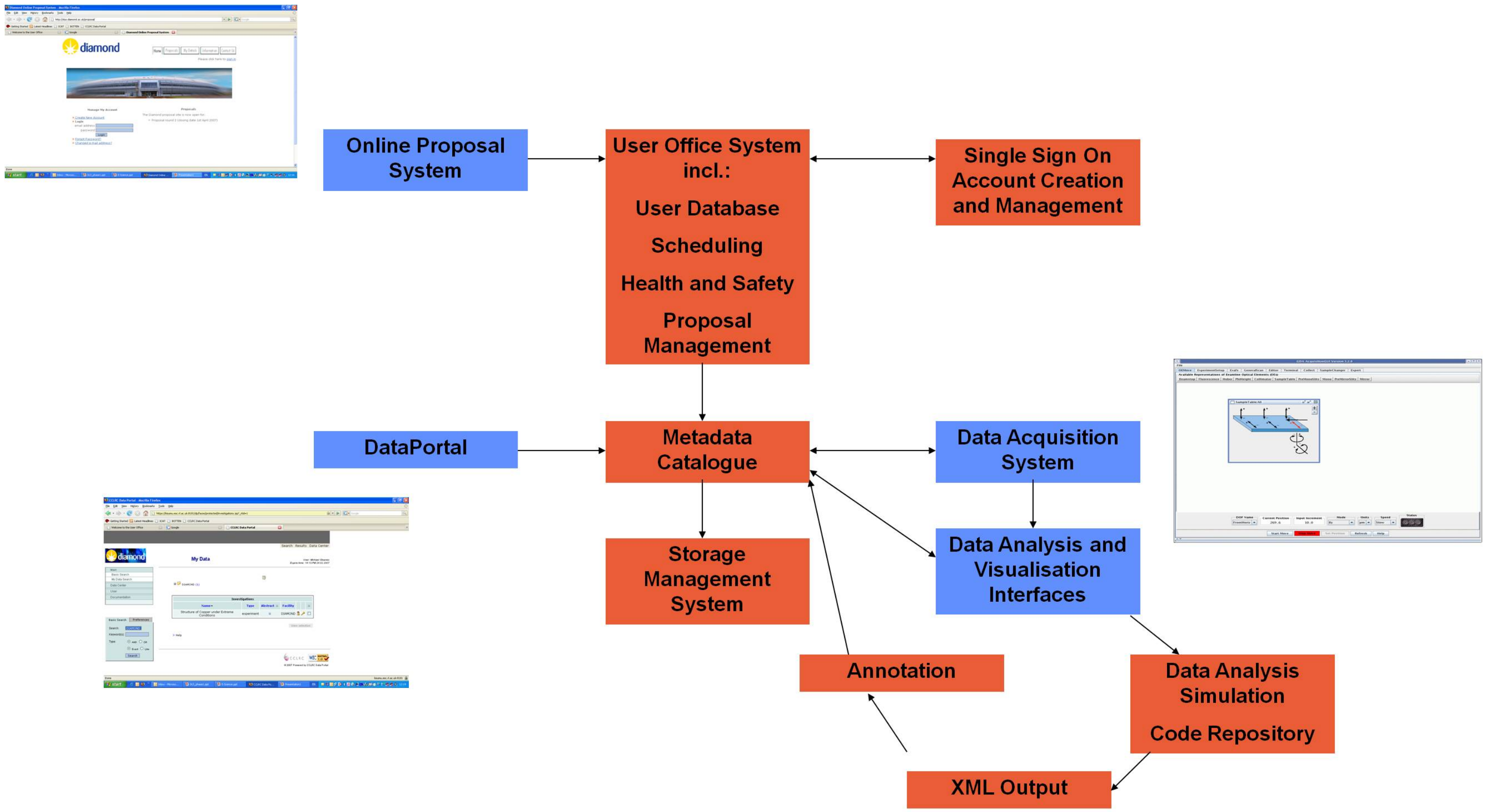
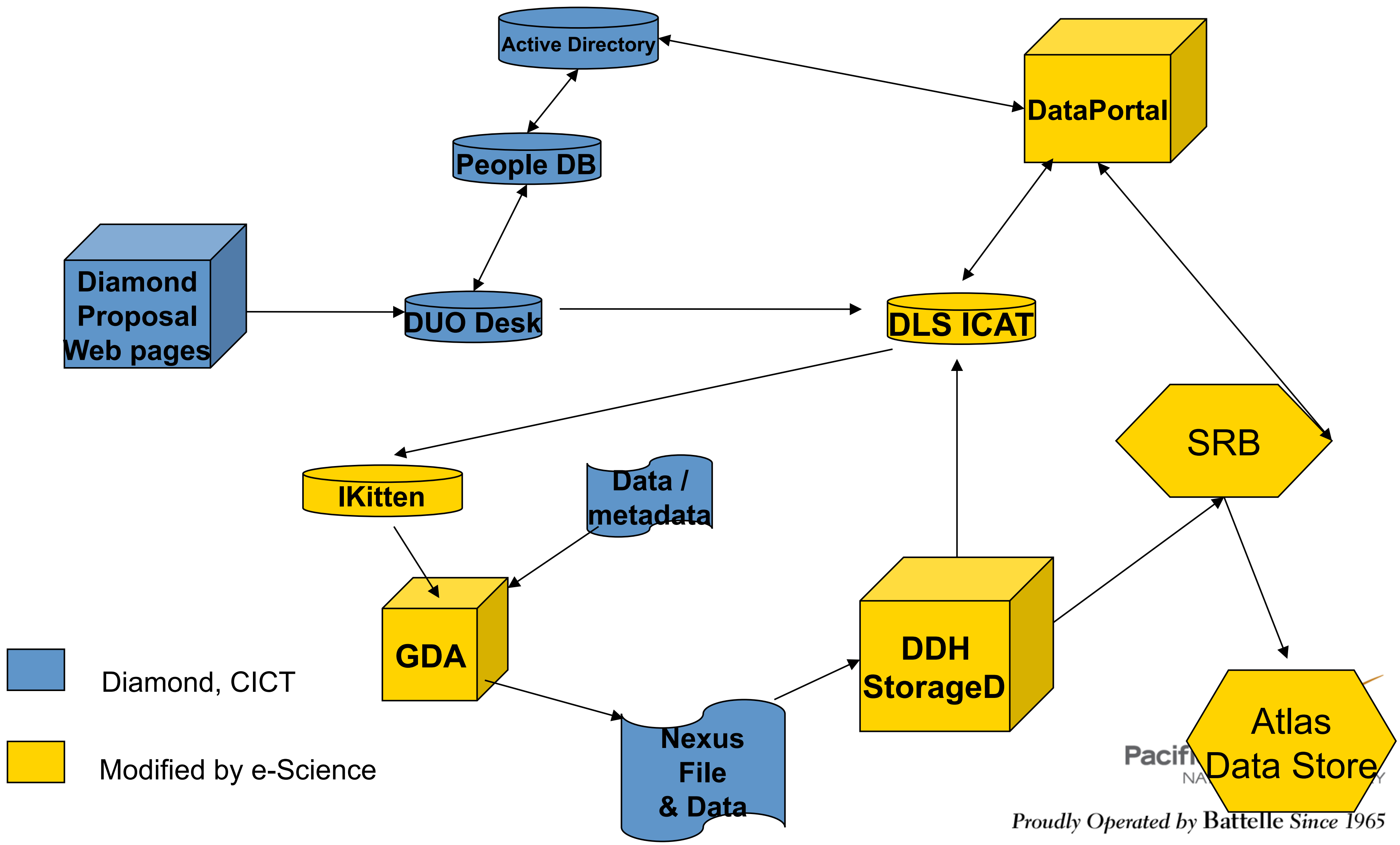
Integrated Infrastructure Architecture



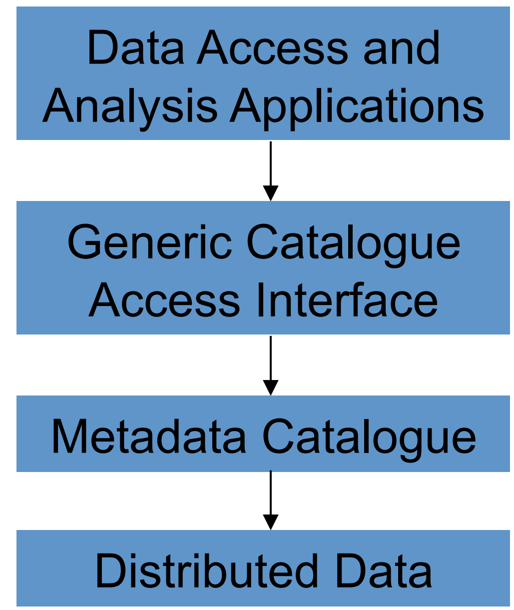
CCLRC Integrated e-Infrastructure for Facilities

DIAMOND Implementation



ICAT Software Suite

- The ICAT software suite centrally catalogues all experiment related information and extracts key results.
- Where ever possible information is gathered automatically trough integration with existing IT systems such as proposal systems or data acquisition.
- The catalogue and the data it references are accessible via a well defined API for easy embedding into any applications.



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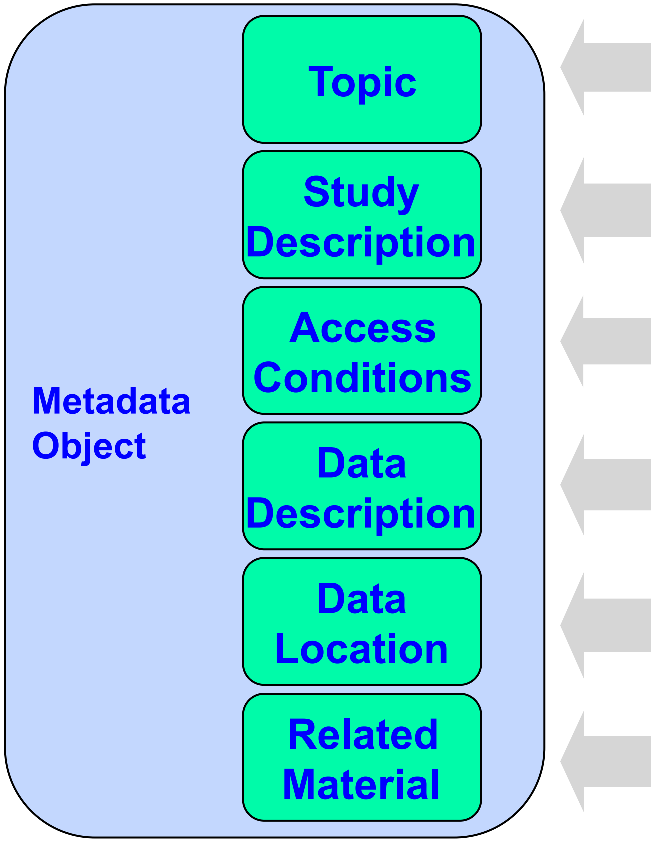
Metadata Model



Keywords providing a index on what the study is about.

Provenance about what the study is, who did it and when.

Conditions of use providing information on who and how the data can be accessed.

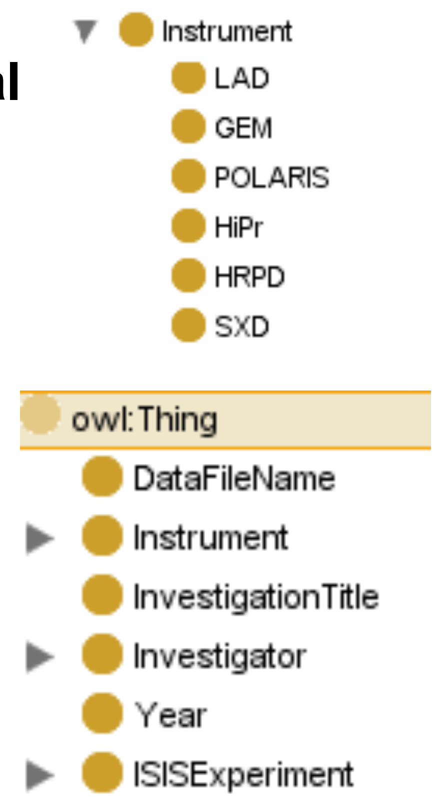
Detailed description of the organisation of the data into datasets and files.

Locations providing a navigational to where the data on the study can be found.

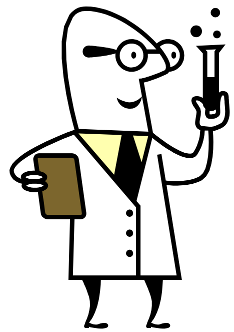
References into the literature and community providing context about the study.

Ontology Support

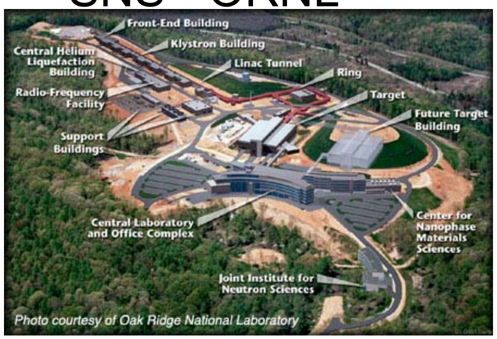
- **1,700,000 distinctive keywords ISIS ICAT**
- **These keywords are used to index experimental studies**
- **The creation of ontology's at ISIS aids the mapping of familiar terms in one domain as well as related concepts in different domains.**
- **Facilitates searching of data by category and grouping of data into keywords across studies. Faster results and enabling of cross facility search.**



Infrastructure – Access to Multiple Facilities



SNS - ORNL



CSL - Canada

Data Portal

ISIS – TS1 + 2

DLS

SRS + ERLP

CLF

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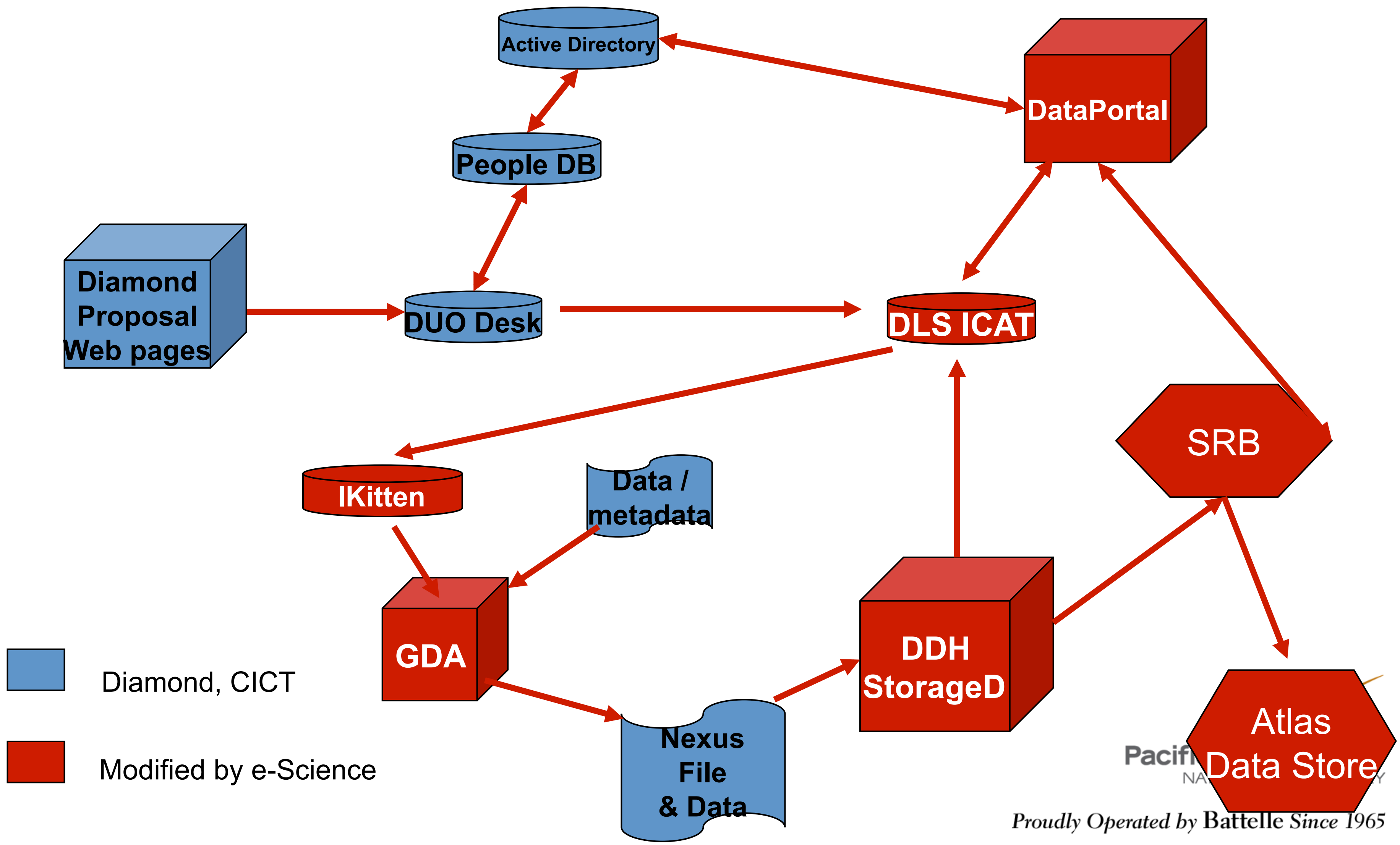
What was achieved by 2008

- Agreed common metadata model, data formats and single sign on allows scientists to have rapid access to their work
- A 20 year back catalogue of ISIS raw data
- All future data collected at STFC Facilities and DLS will be curated and made available for reuse now and in the future
- Raw Data archived and available to project collaborators on- and off site within minutes of collection

Lessons Learned

- **Address Early on:**
  - Resolve institutional and/or personal issues in dealing with mistrust and the use of the data collected
  - Developing agreements, policies and procedures for data governance, ownership, sharing, citations and authorship. How do you reference my data in your publication, agreed embargo times
  - Acknowledge ‘language barriers’ between different project partners
- **Design:**
  - Metadata is the key enabling technology
  - Automation and reliability of processes are vital
  - Interfaces should be as familiar as possible
  - Close integration into existing scientific processes
  - Step wise progression to take users ‘along’

Many Components to Monitor and Control



Automation and Integrated Analysis – MyEMSL 2010

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EMSL

Environmental Molecular Sciences Laboratory:

A national user facility integrating experimental and computational resources for discovery and technological innovation

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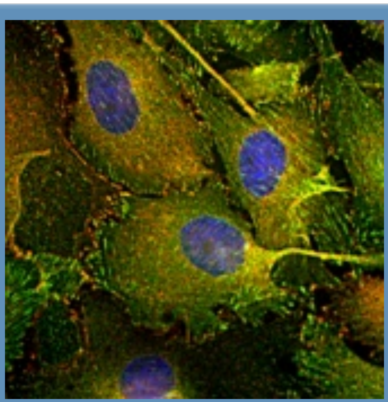
U.S. DEPARTMENT OF ENERGY

The user program is focused on three science themes

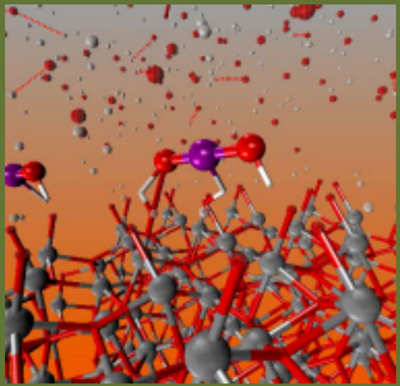
EMSL

Biological Interactions and Dynamics



Understanding and optimizing the response of biological systems to their environment.

Geochemistry/Biogeochemistry & Subsurface Science



Unraveling molecular-level phenomena to determine their impact on contaminant migration and transformation.

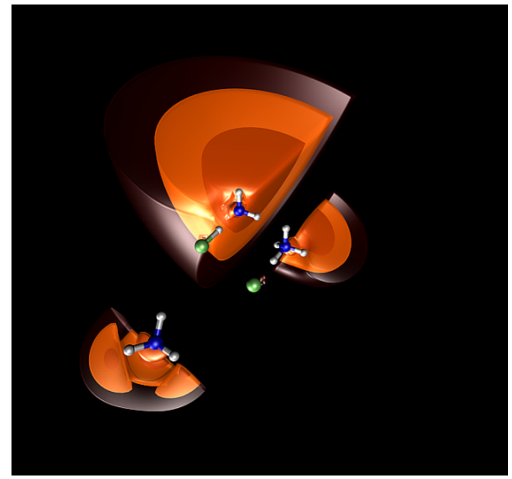
Science of Interfacial Phenomena

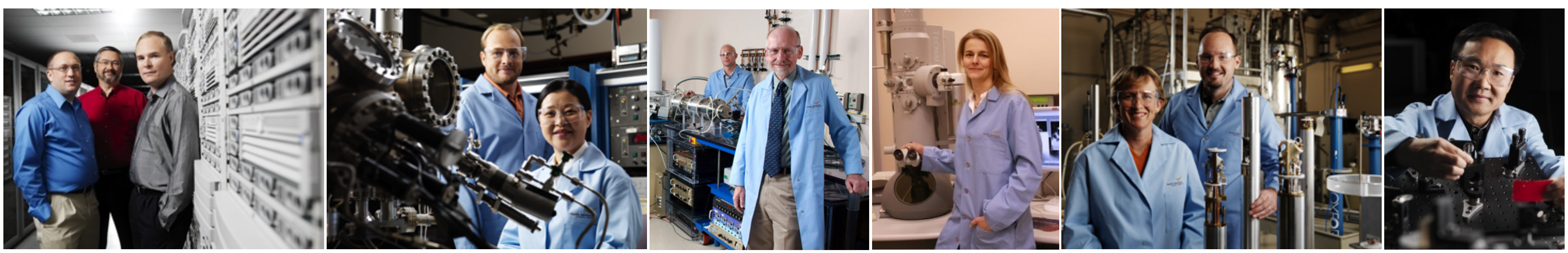
Developing & verifying predictive models for interfacial processes and advancing understanding of structure-function relationships in complex systems.

Capabilities

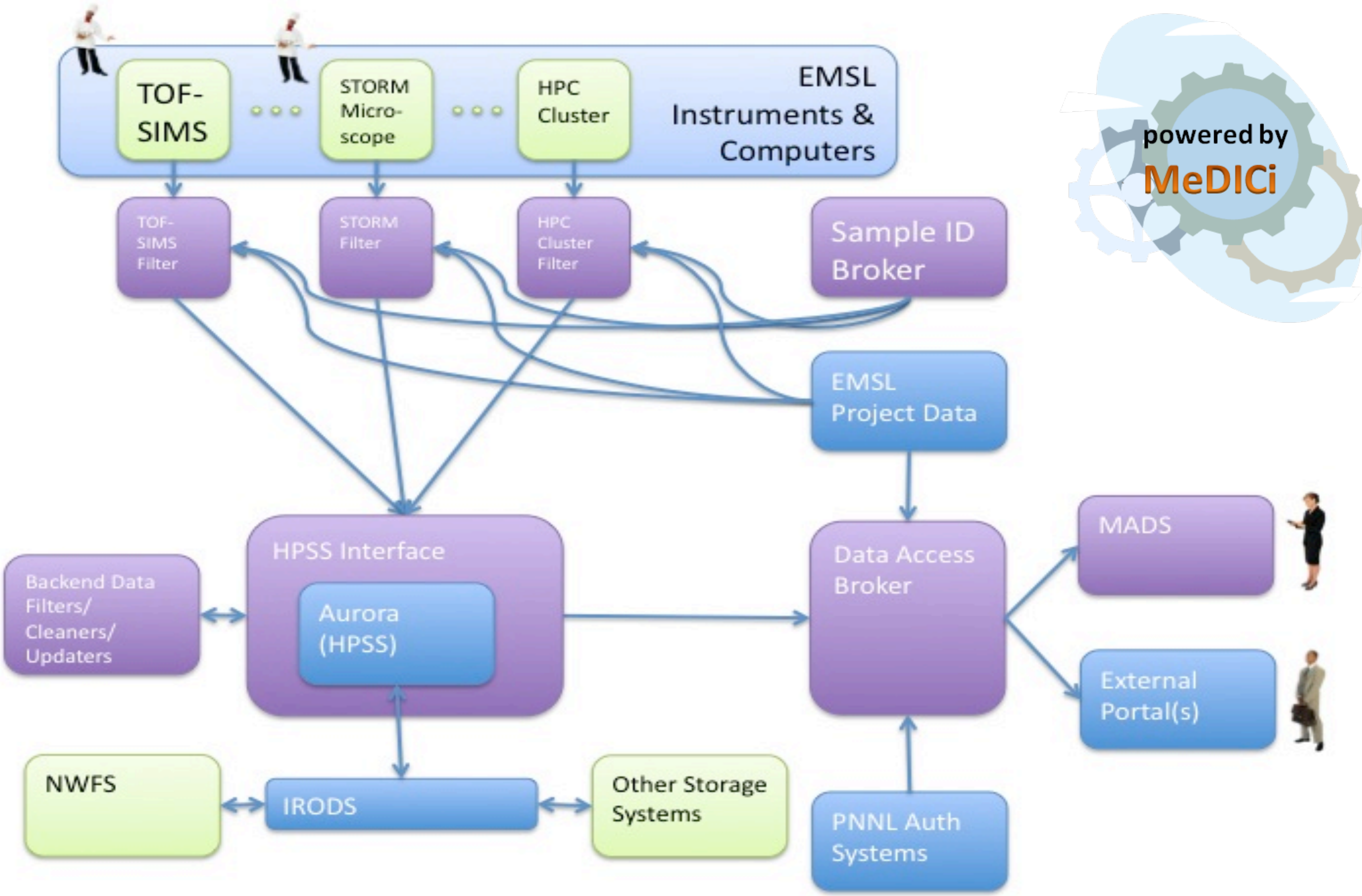
EMSL houses an unparalleled collection of over 100 state-of-the-art imaging capabilities that are used to address scientific challenges:

- Molecular Science Computing
- Deposition and Microfabrication
- Kinetics and Reactions
- Mass Spectrometry
- Microscopy
- NMR and EPR
- Spectroscopy and Diffraction
- Subsurface Flow and Transport





MyEMSL Base Architecture



What is the MeDICi Integration Framework?

EMSL

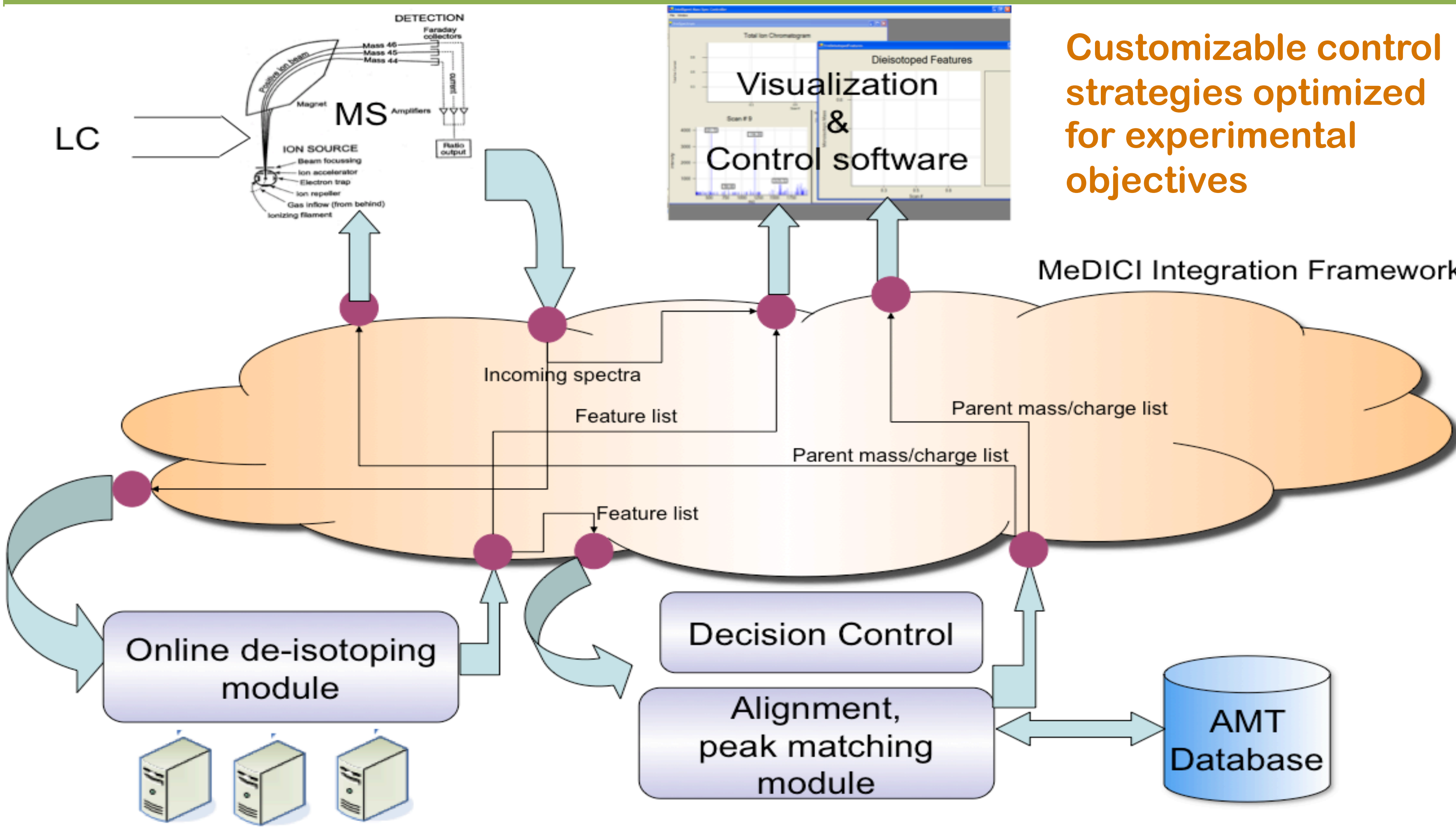
- Java-based integration technology
- Component-based API for creating analytical pipelines
  - Asynchronous component model for Java or non-Java (eg .exe, C/C++, R, Haskell, etc) codes (flexible)
  - Components can be distributed or executed in framework container (scalable through replication/partitioning)
  - Components communicate over a variety of protocols (e.g. JMS, Web Services, sockets, etc.) (configurable)
- Built on robust, industry-tested Java technologies
  - Service-Oriented Architecture (Mule open source ESB)
  - Java Messaging Service (e.g., ActiveMQ,)
- Hooks for provenance capture/workflow orchestration

Smart Instrument Control

High Performance Data Analysis Tools for Intelligent Mass Spectrometer Pipeline

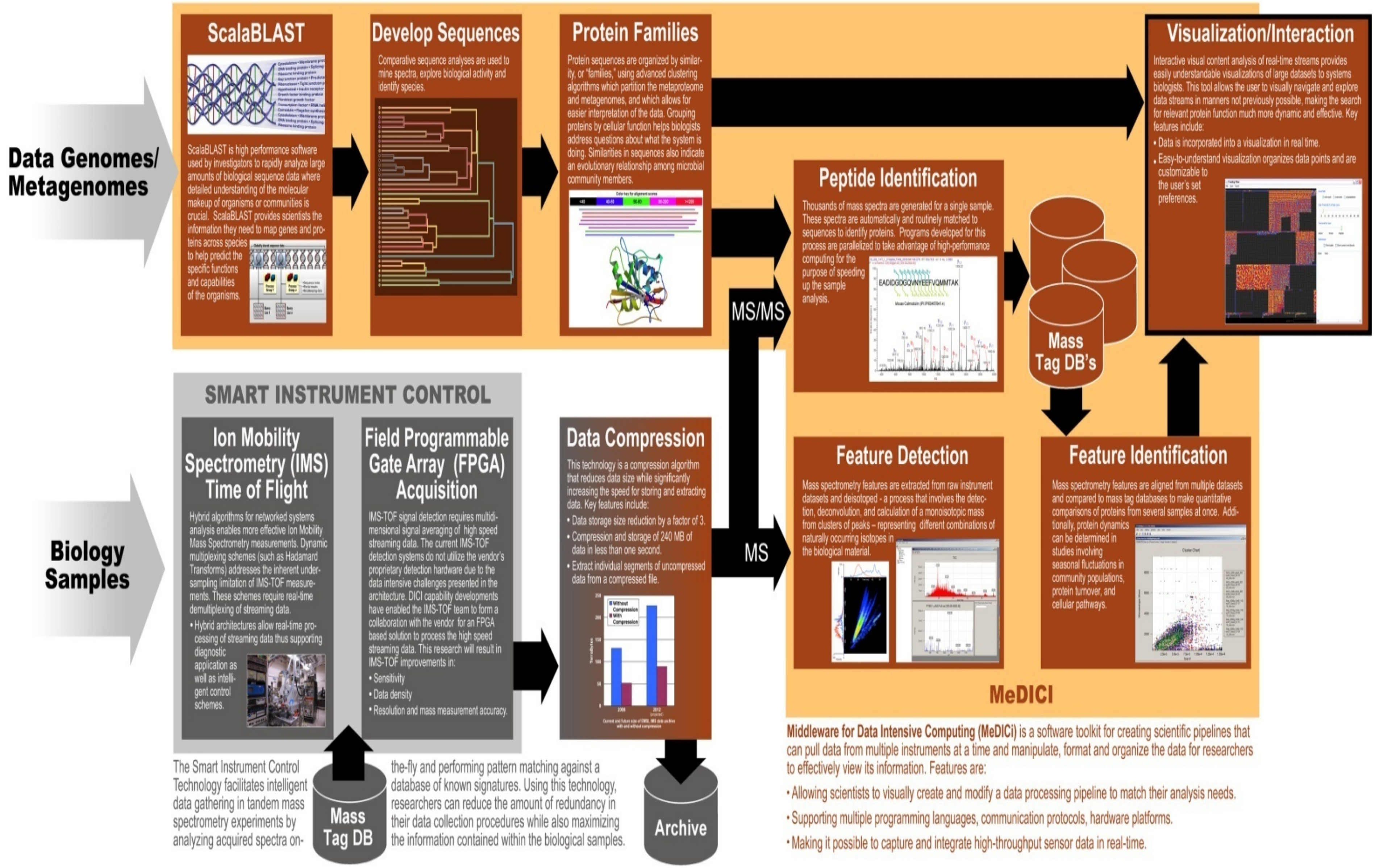
EMSL

Customizable control strategies optimized for experimental objectives



Next Generation Proteomics Pipeline

EMSL



Achieved to Date

- General infrastructure for automated data capture and annotation
- Intelligent Instrument Control linked to data storage and annotation through workflow framework
- Single Instrument automated analysis pipeline seamlessly linked to instrument control, data capture and annotation

Real Time Analysis and Integration – PNNL Chemical Imaging Initiative

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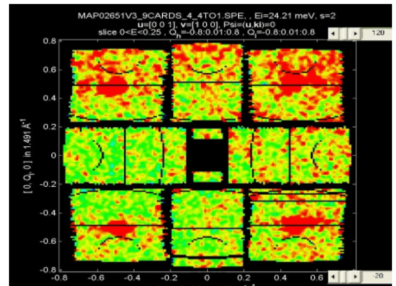
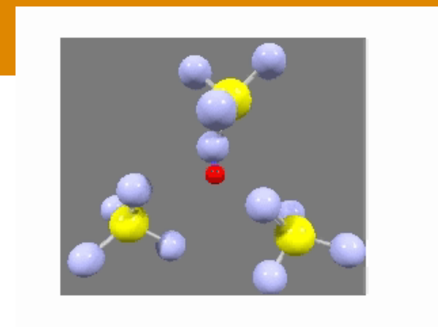
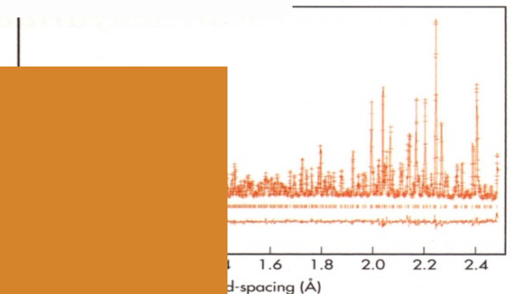
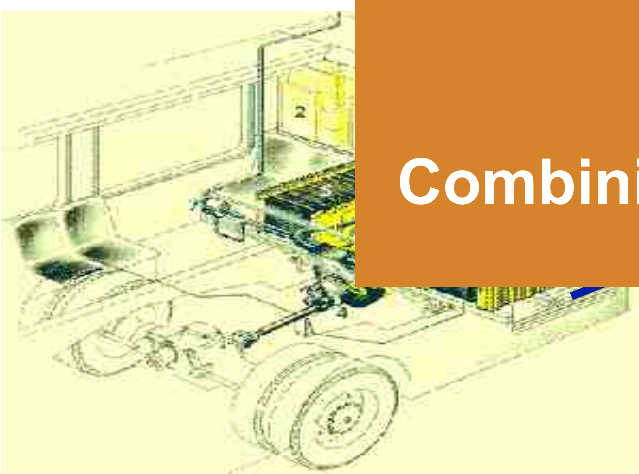
Science needs to answer complex Questions



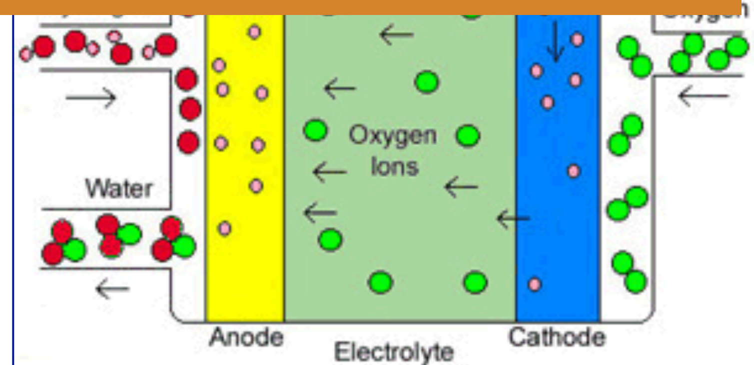






Making it Happen

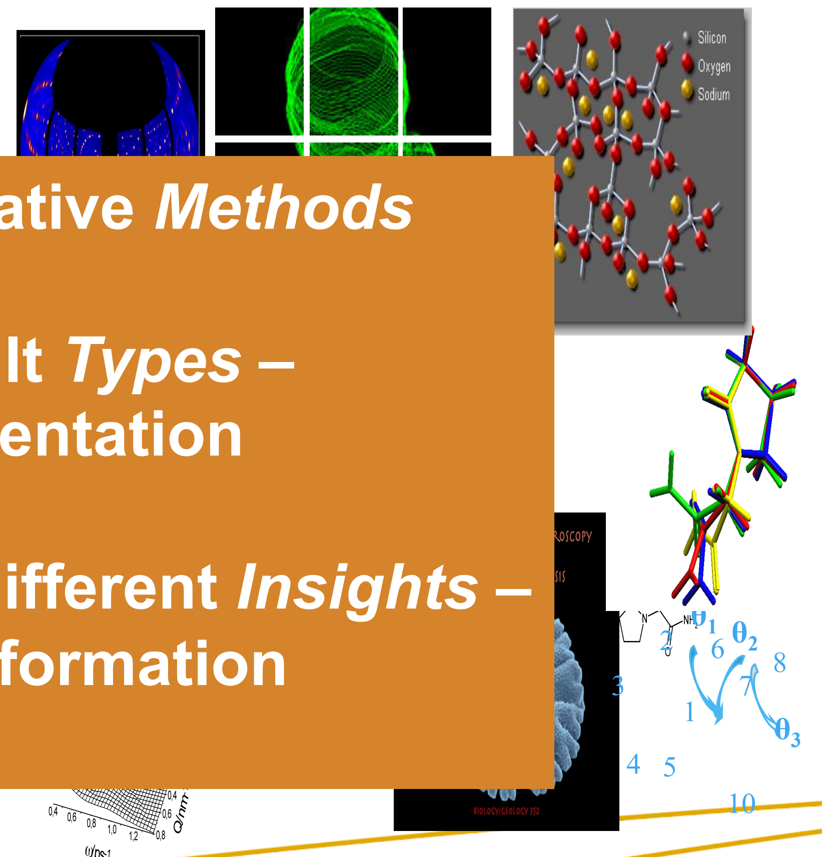
Many People –
Combining complementary Expertise



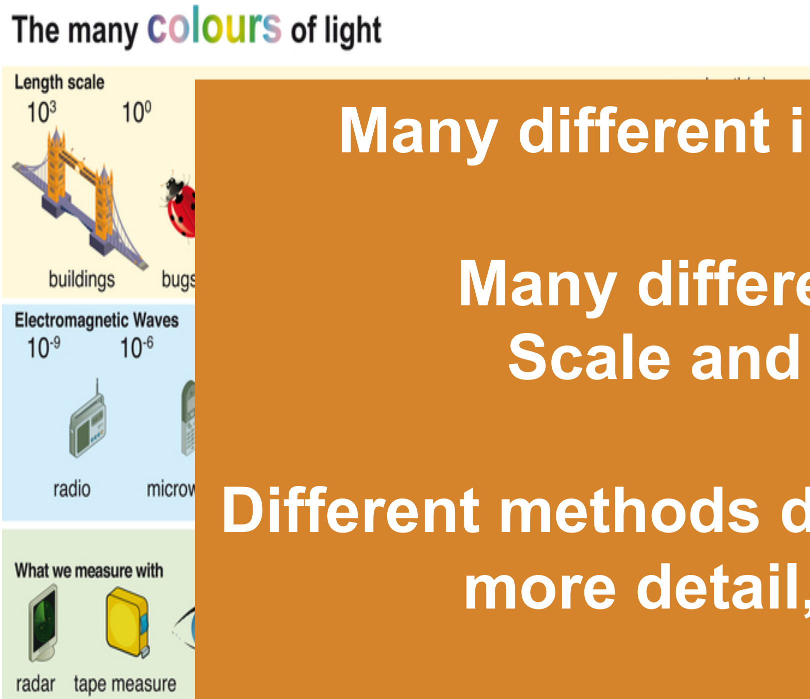
Dr. Robert McGreevy, ISIS, UK

Investigative Methods

Result Representation



Methods



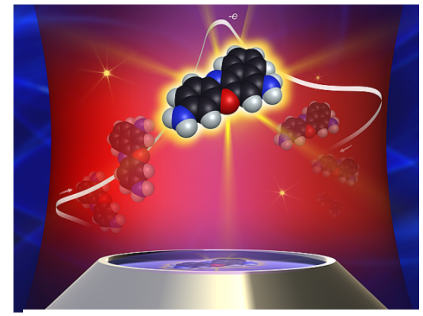
DIAMOND Light Source UK, 2010

Many different investigative *Methods*

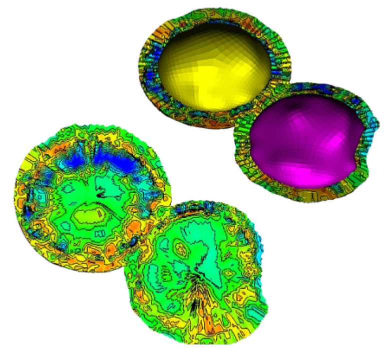
Many different result *Types* –
Scale and Representation

Different methods deliver different *Insights* –
more detail, new information

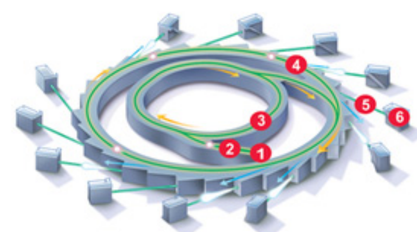
Real-World Manipulation on a Molecular Level



- **Purpose: Deliver a suite of unique tools with nanometer scale resolution and element specificity that will allow researchers to go from model system observation to real-world manipulation on a molecular level.**

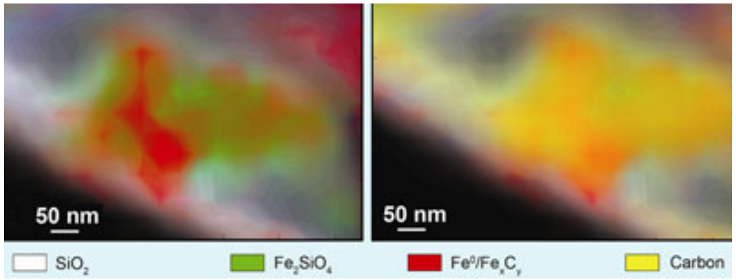


- **Approach: We will build signature, *in-situ* capabilities in**
  - **Light source based x-ray and VUV probes coupled with laboratory based imaging capabilities for 3D tomographic, structural, and element specific interrogation at the molecular level**
  - **Coupled optical, electron, ion, mass, and scanned probe microscopies to understand chemical and biological transformations and mechanisms**
  - **Integrative hardware and software applications for image reconstruction, feature extraction and information integration**

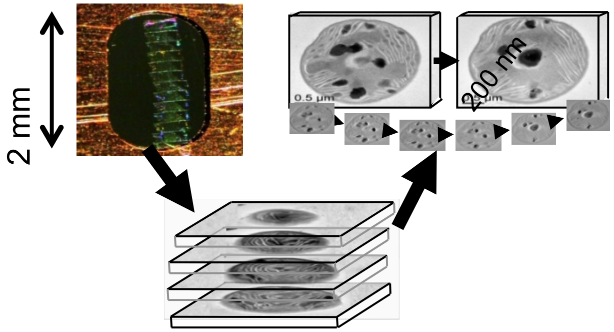


What will allow us to go from model system observation to real world manipulation of *in situ* interfaces on a molecular level?

- **Direct visualization of chemical, material, and biological transformations are essential to achieve a confident level of control over complex systems**
- **Most of our ability to control matter today is through inference and interpretation of spectroscopic and structural data and modeling**
- **Direct Observation: With molecular scale imaging tools and concomitant data handling and analysis methods we can achieve the level of control enabling rational design and synthesis of new chemical, biological, and materials systems.**



Chemical map of a FT catalyst – proto molecular movie

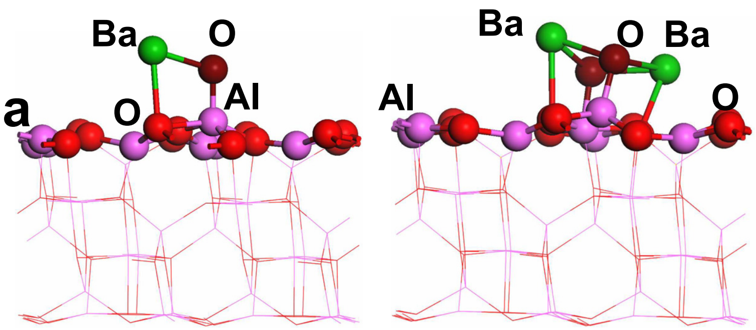


3D EM tomography of Cyanothece Cell

Atomic and Electronic Structure of Catalysts by Combination of In-situ and Ex-situ Imaging

Challenges:

- **Oxide nanoclusters supported by gamma alumina**
  - Physical structure and chemical state of elements
  - Electronic structure
  - Influence of these in catalytic properties



BaO monomer and dimer on a dehydroxylated γ -Al_2O_3(100) surface

Kwak et al, Journal of Catalysis 261, 17-22, 2009

Approach:

- Class of TMO (e.g., WO_3, MO_3, V_2O_5) and TM (e.g., Pt, Cu) supported by g-Al_2O_3 substrate are important
- Combination of in-situ and ex-situ aberration corrected TEM, STEM-HAADF imaging, EDS and EELS spectroscopy
- Integration of high energy resolution EELS measurements with light source XAS
- Integration of experimental data with DFT calculations

Understanding Chemical and Structural Changes in Battery Materials

Challenges:

- **Discovering new materials with high capacity**
  - **- Less volume expansion**
  - **- Enhance charging and discharging rate**
  - **- Less irreversible microstructure formations**

Approach:

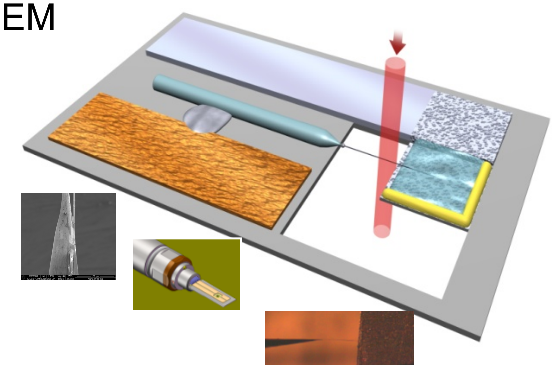
- Combination of nanomaterials and in-situ structural and electrochemical measurements

- Combination of TEM, STEM and APT

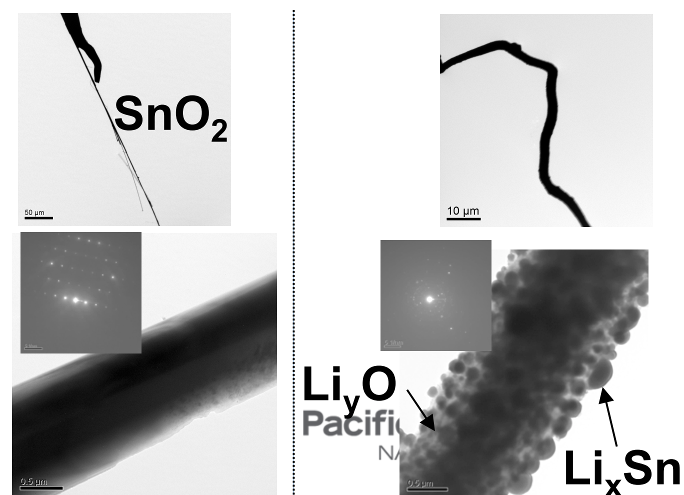
- Integration of high energy resolution EELS measurements with light source XAS techniques – chemical state charge transfer information

- Integration of experimental data with calculations (DFT and MD)

Basic conceptual design of battery using a single nanowire for in-situ TEM



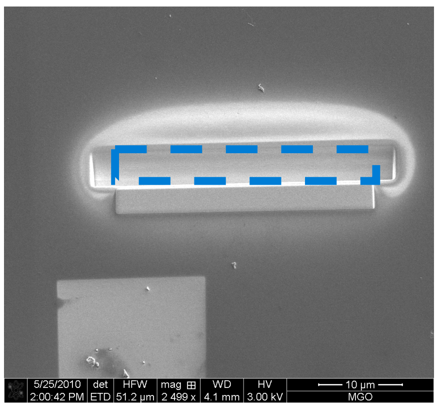
Microstructural evolution of SnO_2 anode upon initial charging



Integrated Sample Preparation and Analysis Platform for Comprehensive 3-D Chemical Imaging

Challenges:

- **Determining 3-D positions and chemical identity of individual atoms in any materials system, analysis across different imaging techniques**

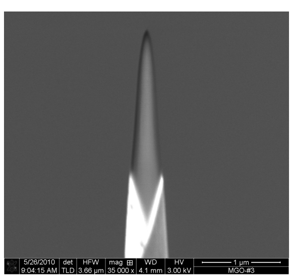


DB-FIB

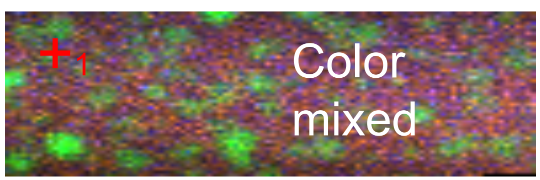
TEM

APT

DB-FIB

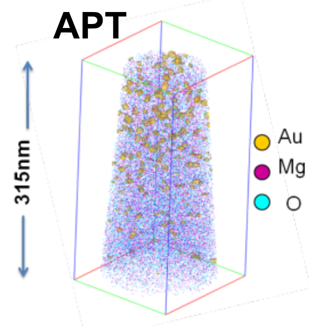


STEM



Mg: Orange
O: Blue
Au: Green

APT

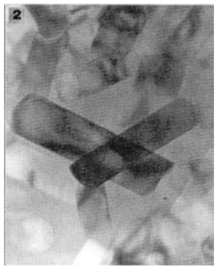


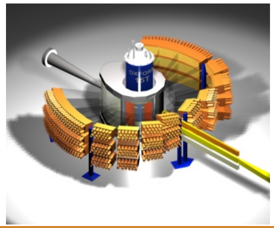
Effectively relating Information and Knowledge

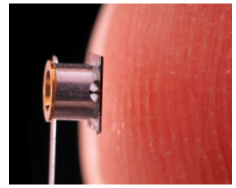
We need a map and plan that describes how things fit together - in specific areas and in the whole

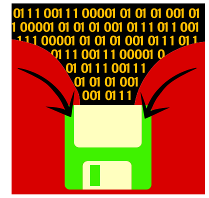
Different people have different perspectives and experiences, expecting information represented in their context

Context sensitive, flexible Framework







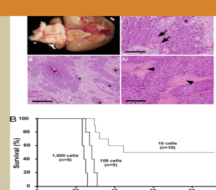


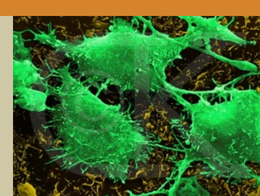
Characterize Different Components

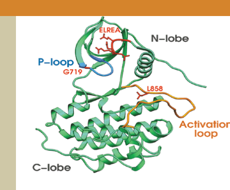
Methods
- •Describe
- •Map
- •Classify

We need a flexible framework that allows scientists to integrate, compare and contrast results from different investigative methods – and presents the results in a context that they are familiar with

Framework
Relating
Comparing
Combining
Synthesizing



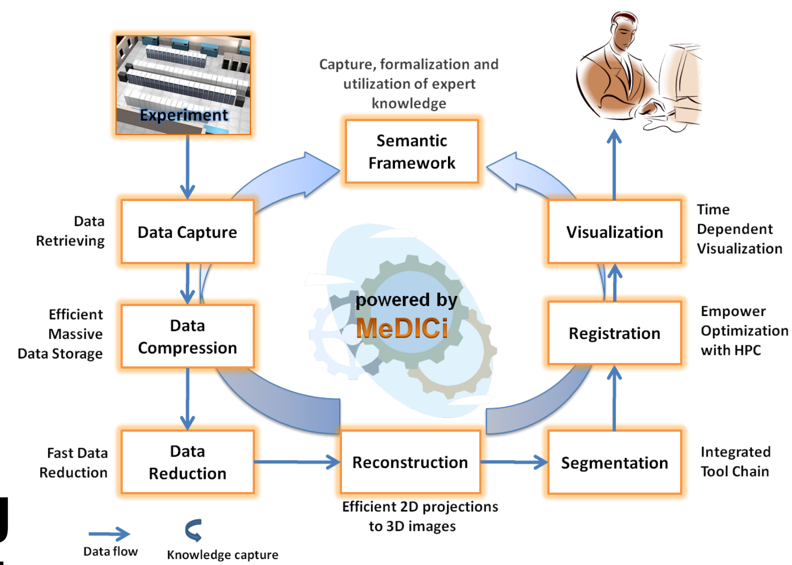




Different View Points – Shared Knowledge

Develop synergistic integration of multiple imaging, characterization, and simulation techniques

- Phase 1: In collaboration with scientists establish basic data analysis and handling framework
- Phase 2: Develop integrative analysis methods across different chemical imaging technologies with support of the wider community
- Phase 3: Evolve data handling and analysis methods to meet the real time and high data volume requirements of the new chemical imaging capabilities



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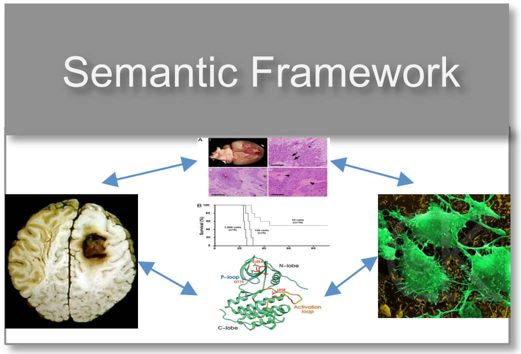
Key Challenges

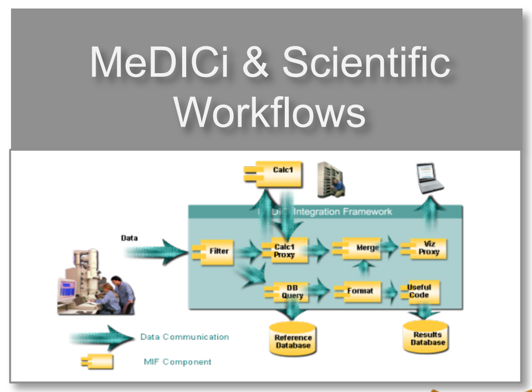
Challenge	Today	Tomorrow	Technologies
High Data Rate	5PB / Year LHC	3.5 PB / Day XFEL	Storage / Movement/ Analysis
Real Time Analysis	After Experiment -18 hours for 3D TEM reconstruction	Experimental Steering through real time analysis during experiment	Real Time, Parallel, Data Intensive Computing HW + SW
Integration across different Imaging Technologies	One off integration of 2 techniques	100's of combinations possible	Conceptual Relation, real time integration
Integrating across scales	On related scales only	Nano to Macro	Conceptual Relation
Geographical distribution of experimental sources to be integrated	None	10's – flexibly combined	Distributed Computing Paradigm

Proposed Core Framework Development (1)



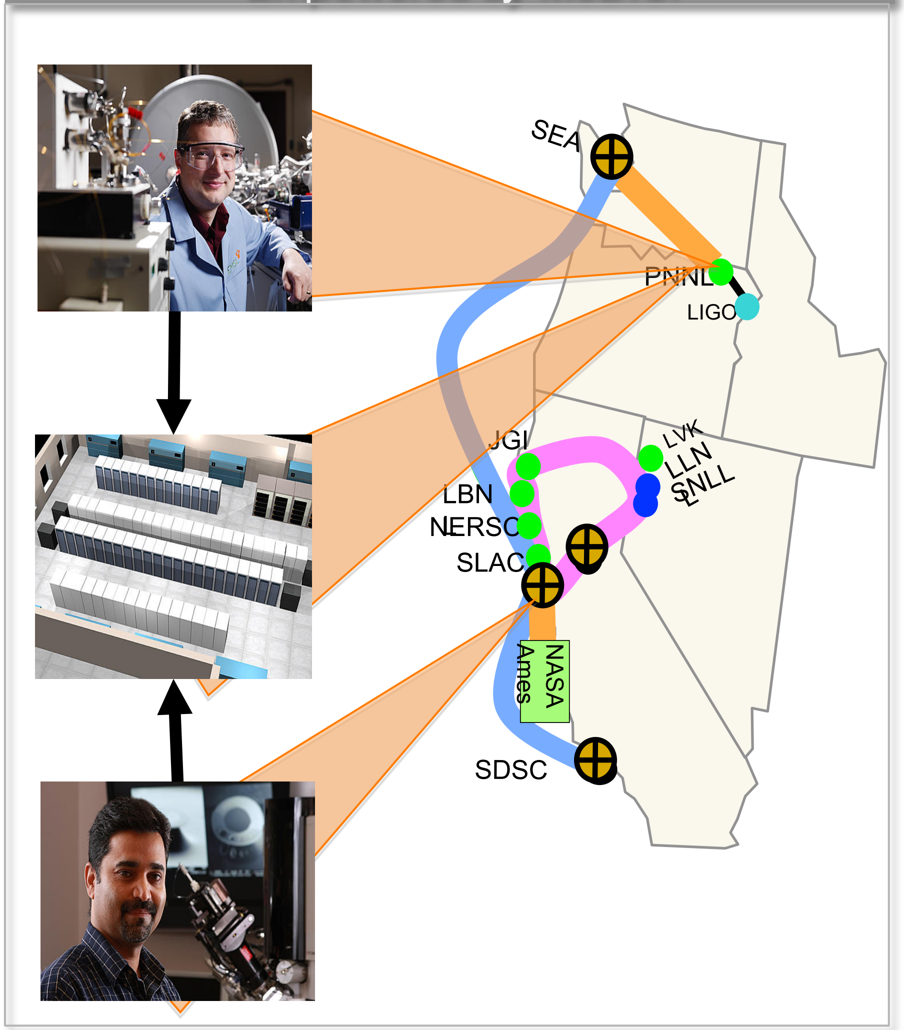
- Formal characterizations of the methods, instruments, samples, analysis processes and associated data products.
- Formalized topology of the methods, their contribution and constraints.

- Flexible creation of data intensive workflows.
- Managing complex and intensive data exchange as well as rapid integration of data sets spanning different spatial and temporal scales



Proposed Core Framework Development

Data Capture and Distributed Computing Empowered by MeDICi



- Leveraging MyEMSL framework providing workflow, data capture, metadata capture, a central data repository, and tools for data discovery.
- High volume data transfers.
- Taking analysis to the data via distributed computing.

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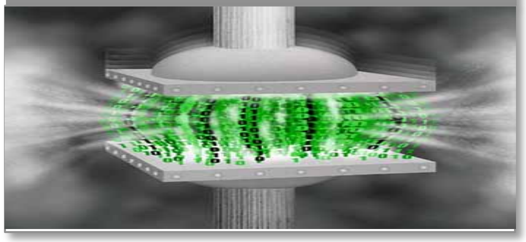
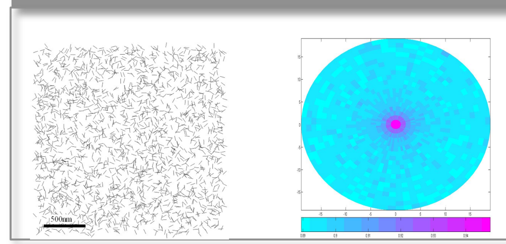
Proposed Example Components (1)

Data Compression



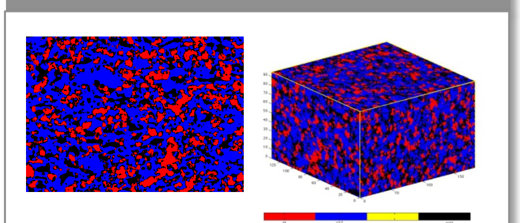
- Appropriate lossless and lossy compression algorithms
- High compression ratio with low computational overhead

Data Reduction



- Reduce noise and smooth data
- Reconstructions will contain the most significant information, are feature-accentuated

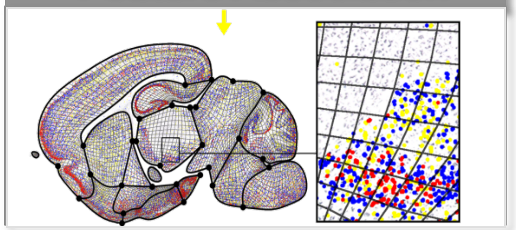
Reconstruction



- Accurate re-construction of high volume data in real time
- Combine correlation functions with parallelized filtered back projection

Proposed Example Components(2)

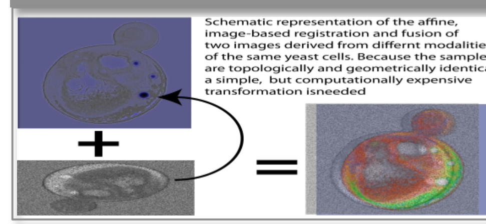
Segmentation & Feature Association



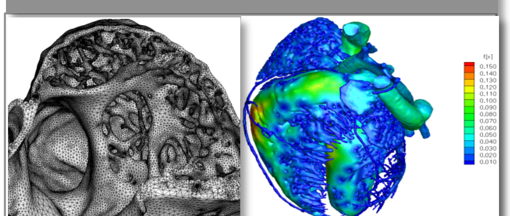
- Scalable differential operators and primitives that can be combined at run time for application-specific chemical signature and feature recognition

- Enabling accurate localized comparisons between experimental datasets from different chemical imaging techniques at high resolutions

Registration



Visualization & Analysis



- Real time, remote, in-situ, high data volume 3+4D visualization

Initial Steps

- **Identification of a small number of key scientific workflows**
- **Determine analysis and integration steps together with scientists**
- **Implement initial end to end workflows to exercise all framework components**
- **Move on to other workflows – test generalization, encourage community involvement**

Questions ?